III.D.2 SOFC Model Development at PNNL

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Objectives

- Develop, improve, and validate modeling tools for analyzing solid oxide fuel cell (SOFC) cells, stacks, and systems.
- Transfer the modeling technology to the Solid State Energy Conversion Alliance (SECA) vertical teams for their use in designing and building SOFC cells, stacks, and systems.
- Conduct training sessions that SECA vertical team members can attend to learn to use the customized modeling tools created.
- Identify degradation mechanisms critical to extended operation and performance of SOFCs, and implement into existing modeling tools.

Approach

- Microstructural level modeling analyzes the flow of chemical species and electrical current within the cell electrodes to determine the effect of microstructure and material defects on electrochemical performance.
- Stack level models investigate the stack geometry and stack component material properties for suitability in creating well-operating and long-lasting designs.
- System models use knowledge of the operating characteristics of cell and stack designs to create optimized environments that will ensure the longest possible life span.

Accomplishments

- Incorporated stack-electrochemistry models, developed at Pacific Northwest National Laboratory (PNNL), into the MARC and STAR-CD codes in the form of Graphical User Interface (GUI) Stack Modeling Tools.
- Validated STAR-CD model temperature predictions with experimental measurements.
- Benchmarked thermal-electrochemical results of the MARC EC implementation against STAR-CD results.
- GUIs presented at the SECA Modeling and Simulation Training Workshop.

Future Directions

- Focus will be on life prediction in the cell and stack level modeling efforts.
- Computational fluid dynamics (CFD) electrochemical (EC): Include submodels to predict the degradation of electrochemical performance over time.
- Finite element EC: Improve geometry options, flow field characterization, and structural evaluations in the MARC GUI.
- Evaluate seal damage and thermal cycling effects in stack level models.
- Evaluate transient response of the controls/system model.

Introduction

Modeling tools have been developed under the SECA Core Technology Program to aid industrial teams in design and analysis of their SOFC designs in several areas. The bulk of the work in SOFC modeling has centered primarily on flow-thermal-electrochemistry behavior using a computational fluid dynamics (CFD) approach. This has been very successful in design of flow fields for planar stacks, where critical metrics are power density and temperature distributions. These temperature results have then been used as inputs for structural models to assess stack mechanical stresses. These models have been useful in designing the physical support for the electrodes (e.g., edge-to-edge and frame-supported electrodes) and rigid glass seals for air and fuel gases. For example, the combined use of these tools demonstrated the advantage of the co-flow design, which is more structurally robust as a consequence of its lower temperature gradients. These modeling tools have been critical for developing a "working" product and evaluating relative performance of stack designs under steady-state conditions with virgin materials properties.

Approach

In the current year, work has been directed to 1) migrate tools for the CFD electrochemistry evaluation into a finite element framework, 2) extend tools to evaluate degradation, and 3) create tools for studying system integration. This first task uses finite element numerical procedures to obtain results adequate for engineering design of stacks. Specifically, by using assumed or approximated flow fields, a multi-physics solution for both electrochemistry and structural response can be obtained within a single software application, with less computational effort due to greater numerical efficiency. This is done using MSC's MARC code. The second major task is building on the existing tools for short-term performance to address the potential degradation mechanisms in the stack. To address this subject, relevant degradation behaviors are identified and prioritized according to influence. These are implemented in the models at several levels. On the microscopic level, for example, the effects of fractures on electrochemical processes and mechanical integrity are being investigated. At the macroscopic level, routines will be integrated to assess the influence of the degradation mechanisms at the stack level. Therefore, degradation behaviors can be treated at both a rigorous fundamental level to understand their rates, severity, mechanisms, etc., and also at the stack level to assess overall influence on performance of a particular design. The third thrust is at a higher system level. In field applications, the stack must now interact with accessory equipment and actual electrical loads. Coupled interactions of the fuel cell, the power electronics, and the loads are largely unknown but could potentially have significant effect on cell efficiency and lifetime. System models that capture these interactions will be needed to aid industrial teams with implementation into actual power systems.

Results

Electrochemistry models have long been used in stack level analysis at PNNL with the STAR-CD computational fluid dynamics code. Model results for stack temperatures were validated against experimental results with good correlation. A photo of a one-cell stack test setup is shown in Figure 1. During the stack tests, the inflow and outflow gas temperatures were monitored as the stack generated 44 watts of power at 0.7 volts. A 3-dimensional

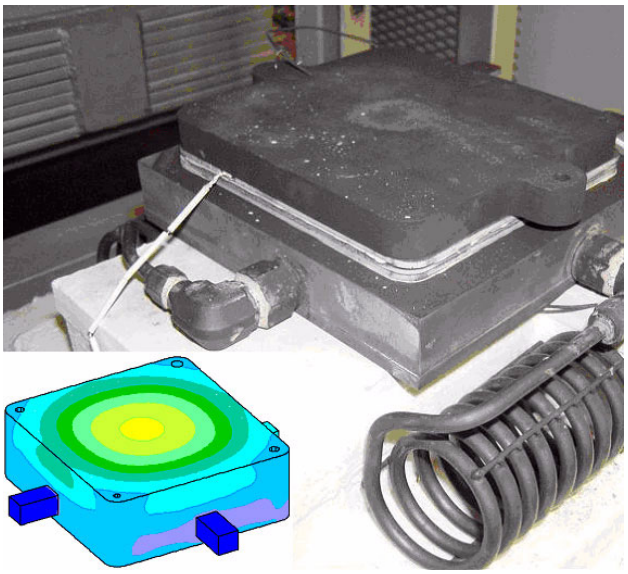

Figure 1. One-Cell Stack Experimental Setup, and the CFD Model Created to Simulate the Experiment (inset)

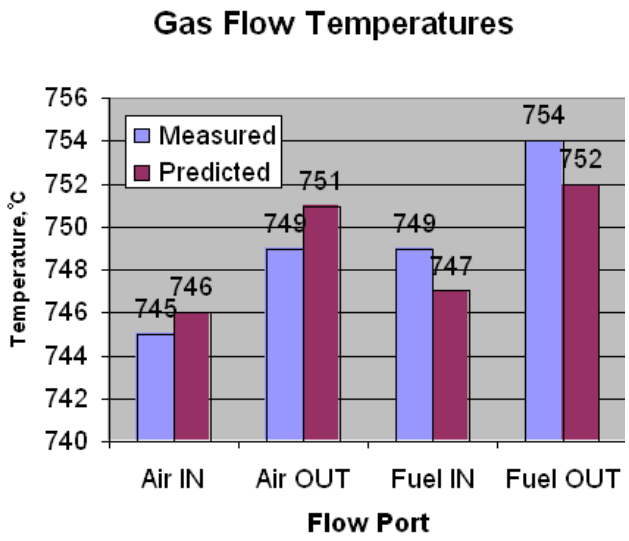

Figure 2. Comparison of Measured and Model-Predicted Inflow and Outflow Gas Temperatures

model of the stack containing 89,000 computational elements was created to mimic the experimental setup (Figure 1 inset). The model predicted inflow and outflow gas temperatures to within 2 degrees Celsius of those measured at the tested power and voltage. A graphic of the measured and predicted temperatures is given in Figure 2.

This modeling capability was successfully migrated into the finite element code MARC. The EC module was developed to calculate the current density distribution, heat generation, and fuel/oxidant species concentrations for a planar cell based on the thermal state, flow conditions, and user-defined electrochemical parameters (Khaleel et al 2004). The output heat generation profile from the EC module is input to MARC, which performs a thermal analysis and iteratively updates the temperature field until the steady-state solution is achieved. The steady-state temperature field can then be further used to obtain mechanical stresses in the stack.

Steady-state results from the MARC EC model were compared with similar STAR-CD simulation results. The case chosen was a cross-flow design with 116.6 cm^2 active area. The cell was operating at 40 watts and 0.7 volts. Fuel and air delivery rates were 4.236E-4 mol/s and 1.69E-4 mol/s respectively. The cell temperature distribution calculated by the STAR-CD stack modeling tool is shown in Figure 3. The cell temperature distribution calculated by the

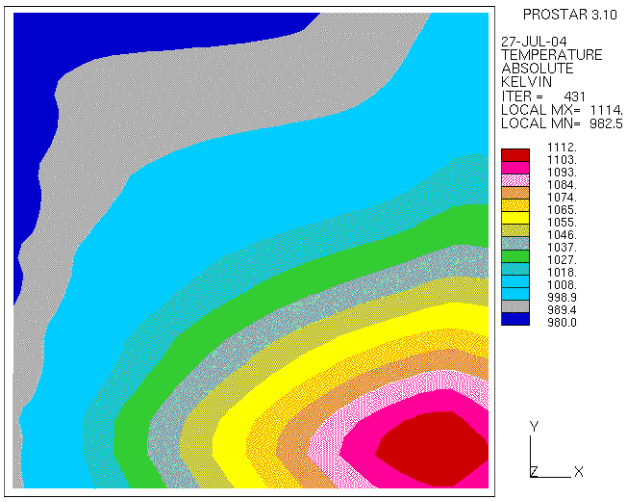

Figure 3. Cell temperature distribution calculated by the STAR-CD stack modeling tool. Cell with 116.6 cm^2 active area operating at 40 W and 0.7 V. Fuel and air delivery rates were 4.236E-4 mol/s and 1.69E-4 mol/s, respectively.

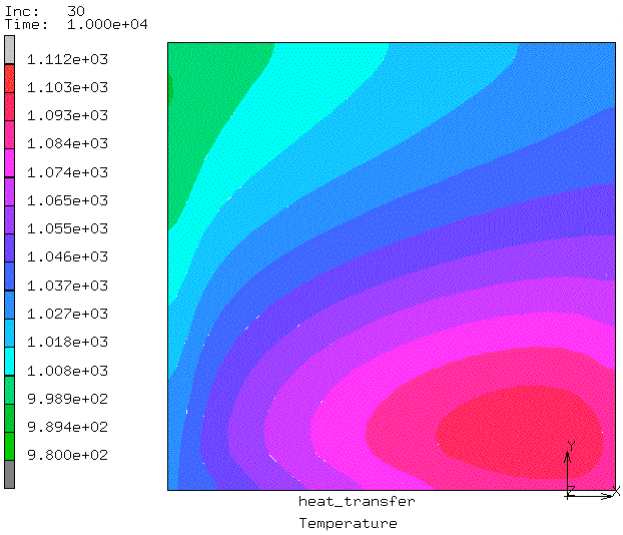

Figure 4. Cell temperature distribution calculated by the MSC stack modeling tool. Cell with 116.6 cm^2 active area operating at 40 W and 0.7 V. Fuel and air delivery rates were 4.236E-4 mol/s and 1.69E-4 mol/s, respectively.

MSC stack modeling tool is shown in Figure 4. Obtaining the close agreement shown in Figures 3 and 4 required adjusting the fuel concentrations in the MARC EC simulation to account for gas diffusion in the inlet fuel stream. The initial comparisons between MARC EC and Star-CD

showed considerable difference between the results until the inlet fuel concentrations were compared. The Star-CD solution includes diffusion of the fuel species in the flow simulation, whereas the MARC EC module assumes that the initial fuel concentrations exists at the inlet edge of the positive-electrolyte-negative (PEN). Closer review of the Star-CD results showed a significant diffusion gradient from the inlet manifold to the leading edge of the active area of the cell. A diffusion approximation (based on a path length from the inlet manifold to the cell, the fuel flow velocity, and the binary gas diffusion coefficients) is being developed to account for this effect.

Specialized GUIs to analyze electrochemical performance of multi-cell planar stacks were created in both the CFD and finite element analysis (FEA) frameworks. PNNL provided technical input to CD-Adapco as they created their customized GUI within STAR-CD and to MSC Software as they developed their customized GUI within MARC Mentat. Both implementations are based on the electrochemical routines developed at PNNL.

The STAR-CD stack modeling GUI has the capability to import user-defined model geometry or use templates to build custom planar cross-, co-, and counter-flow SOFC stack designs. The MARC GUI currently uses a template to build a customized planar SOFC stack design. Boundary conditions and electrochemical performance parameters can then be set and the fuel cell simulation performed. This capability enables the modeler/engineer to easily perform parametric studies of stack performance. Modelers from the SECA industrial partners and from universities were trained how to use this modeling capability by representatives of CD-Adapco (STAR-CD) and MSC Software (MARC) in July of 2004. The PNNL-hosted "SECA Modeling and Simulation Training Workshop" was organized to allow the software companies one full day to train the modelers how to use their "general purpose" baseline code as well as the SOFC-specific GUI. In the training workshop, the modelers had "hands on" use of the tools and provided direct feedback to the software company representatives about the functionality of the GUI as they worked through the training examples and manuals.

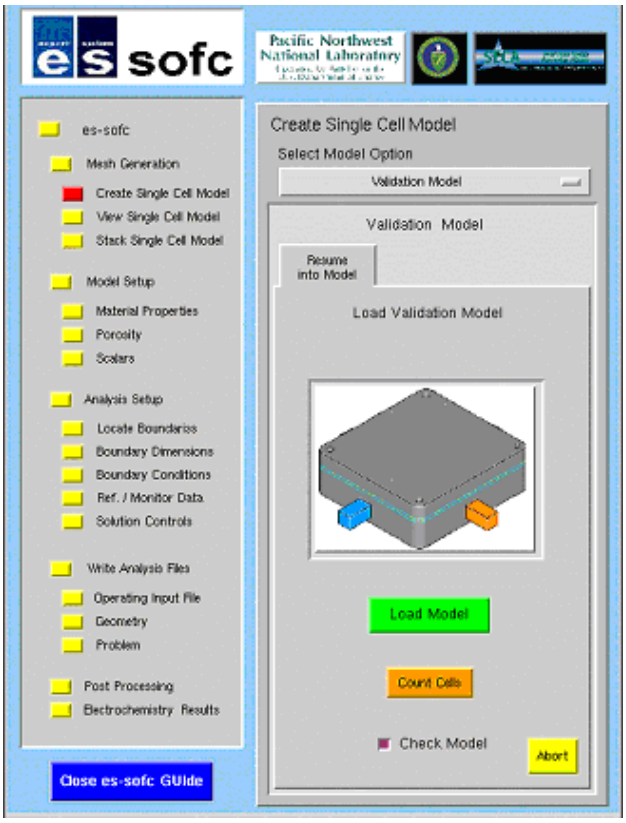

Figure 5. Main Model Setup Window of the STAR-CD GUI named ES-SOFC

The main model setup page for the STAR-CD GUI, named ES-SOFC, is shown in Figure 5. The models are set up step-by-step by working down through the list of tasks in the window shown. Each of the buttons on the list invokes popup windows that prompt the user for input. When the user completes the last step on the main page, the model setup is complete and is ready to run. The MARC GUI main window is shown in Figure 6. Similar to the ES-SOFC window, the models are set up step-by-step by following popup windows that prompt the user for model input. When input is completed, the model is saved and ready to run. In addition to the thermal-electrochemical performance, the MARC model can also be solved to evaluate the temperature-induced mechanical stresses in the cell.

In other activities, enhancements to existing modeling tools were made. On-cell steam methane reforming capabilities were added to the CFD electrochemistry model. This capability will be exercised to provide guidance for optimizing SOFC

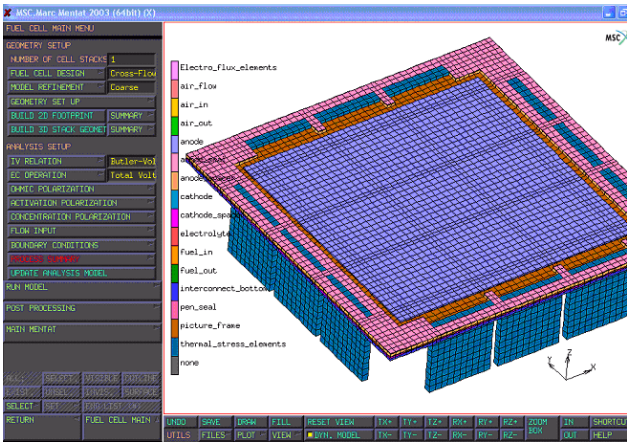

Figure 6. Main Model Setup Window of the MARC GUI

systems with respect to external reformer and blower sizes and the thermal load. For the structural model in MARC, compressive seal behavior was captured using specialized gasket elements and contact surfaces to evaluate the seal contact pressure distribution. Mechanical testing of seals was initiated to fill a void for fundamental material properties and provide mechanical properties and strengths for common seal materials. The data will also be included in the planned materials database. Testing of sealing glass is ongoing, but its inelastic response at cell operating temperatures has been observed.

New modeling efforts have also been initiated. As a basis for the study of cell/stack degradation, PNNL cataloged critical degradation mechanisms, physical parameters, and performance effects for SOFCs. The effect of fractures on electrochemical and mechanical behavior was one mechanism of interest. Microstructural electrochemistry models were used to determine the effect of anode cracks on cell power density, and a continuum damage model was created in MARC to analyze structural integrity of rigid glass seals. These models will be integrated into the higher-level stack models. PNNL has also developed a Matlab/Simulink model of a complete SOFC power system, including the fuel cell, reformer, heat exchangers, battery, controllers, and power electronics. Transient stack behavior in the model was improved by experimental testing of electrical response to load switching.

Conclusions

Advanced computational modeling tools are being developed at PNNL and disseminated to SECA members to aid in meeting required SOFC performance targets.

FY 2004 Publications/Presentations

1. JE Deibler, KP Recknagle, and MA Khaleel, "Modeling of SOFC Stacks in Transition from Startup to Steady State Operation at PNNL," 2003 Fuel Cell Seminar Proceedings.

2. MA Khaleel, Z Lin, P Singh, W Surdoval, and D Collins, "A Finite Element Analysis Modeling Tool for Solid Oxide Fuel Cell Development: Coupled Electrochemistry, Thermal and Flow Analysis in MARC," Journal of Power Sources, Vol. 130, pp. 136-148 (2004).

3. MA Khaleel, KP Recknagle, Z Lin, BJ Koeppel, SJ Moorehead, KI Johnson, N Nguyen, D Rector, and G Grant, "SECA Core Program- Recent Development of Modeling Activities at PNNL," SECA CTP Program Review, May 11-13, Boston, MA (2004).